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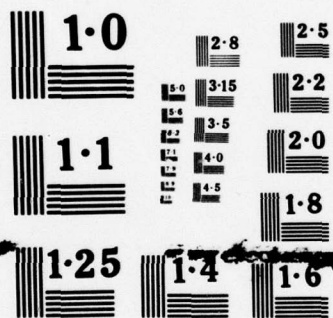
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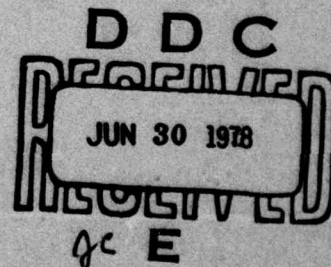
TECHNICAL REPORT MIT-89-PU

## EXPERIMENTAL AND THEORETICAL STUDIES OF CHEMICAL DYNAMICS AND INSTABILITIES IN IRREVERSIBLE PROCESSES

by

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MAY 1978

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Technical Report MIT-89-PU

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AS RELATED TO JET PROPULSION  
OFFICE OF NAVAL RESEARCH, DEPARTMENT OF THE NAVY

CONTRACT N00014-75-C-1143 NR-098-038

EXPERIMENTAL AND THEORETICAL STUDIES OF CHEMICAL  
DYNAMICS AND INSTABILITIES IN IRREVERSIBLE PROCESSES

by

John Ross and F. G. Keyes  
Chemistry Department  
Massachusetts Institute of Technology  
Cambridge, Massachusetts 02139

May 1978

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# ABSTRACT

The final report summarizes the work accomplished under the subcontract. The overall objectives of the investigation were as follows: The determination of molecular properties of chemical dynamics for reactions of importance to combustion and propulsion. Molecular beam techniques were used for the experimental part of this work and were accompanied by theoretical studies in chemical dynamics. The second purpose was the study of the interaction of chemical reactions with transport processes and flows in gases in which instabilities may occur.

## PROJECT SQUID FINAL REPORT

### A. Identification

Principal Investigator: John Ross, F.G. Keyes Professor of Chemistry

Contractor: Massachusetts Institute of Technology

Contract No.: Sub 4965-10 under Contract N00014-67-0226-0005

Title: Experimental and Theoretical Studies of  
Chemical Dynamics and Instabilities in  
Irreversible Processes

### B. Duration:

October 1, 1967 - December 31, 1977

### C. Participation

Other Support: Work has been supported in part by the  
National Science Foundation (30%) and  
M.I. T. (20%).

Names of Investigators  
who contributed to research:

† Robert K. Brown	* Jennifer Makowski
* Randolph H. Burton	* David L. McFadden
Rashmikant C. Desai	Charles Mims
* Michele Flicker	Abraham Nitzan
George P. Flynn	Peter Ortoleva
* John A. Gracki	* Lawrence G. Piper
Hong-sup Hahn	Itamar Procaccia
Raymond Kapral	George Schatz

† M. A.

\* Ph. D.



#### D. Object

**Purpose of Research:** The determination of molecular properties of chemical dynamics for reactions of importance to combustion and propulsion. Molecular beam techniques were used for the experimental part of this work and were accompanied by theoretical studies in chemical dynamics. The second purpose was the study of the interaction of chemical reactions with transport processes and flows in gases in which instabilities may occur.

#### E. Achievement

Extensive progress has been made in the study of chemical dynamics both experimentally and theoretically. We developed simple but effective methods of estimating reaction cross sections which include the details of rotational and vibrational distribution of the energy of reaction in the reaction products.

The study of chemical instabilities proceeded along both theoretical and experimental lines. We demonstrated the theoretical feasibility of a large number of new phenomena such as light-induced spatial structures, chemical oscillations, and multiple stationary states. On the enclosed publication list, research sponsored in part by Project SQUID is marked with an asterisk.



Publications of Professor John Ross

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**To be submitted:**

**"The reaction of photo-excited  $\text{NO}_2$  with Cyclopropane," to be submitted to J. Chem. Phys. (with N. Presser, H. Petek and G. Eadens).**

**"Formation of spatial structures in illuminated systems," to be submitted to J. Chem. Phys. (with K. Iwamoto and N. Presser).**